Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Scalable kinetics treatment for gas–aerosol systems in atmospheric models

Matthew Dawson[1], Matthew West[2], Nicole Riemer[3], and Oriol Jorba[1]

1. Earth Sciences, Barcelona Supercomputing Center, Barcelona, Spain.
2. Mechanical Science & Engineering, University of Illinois at Urbana–Champaign, USA.
3. Atmospheric Sciences, University of Illinois at Urbana–Champaign, USA.

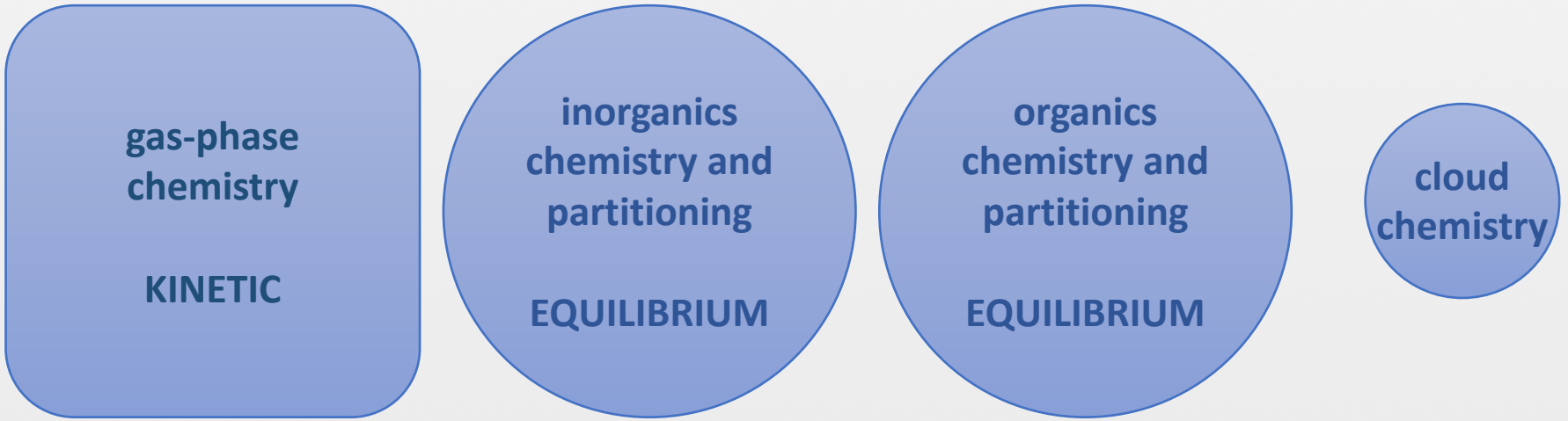
Photography encouraged

10/4/2019

EGU General Assembly 2019

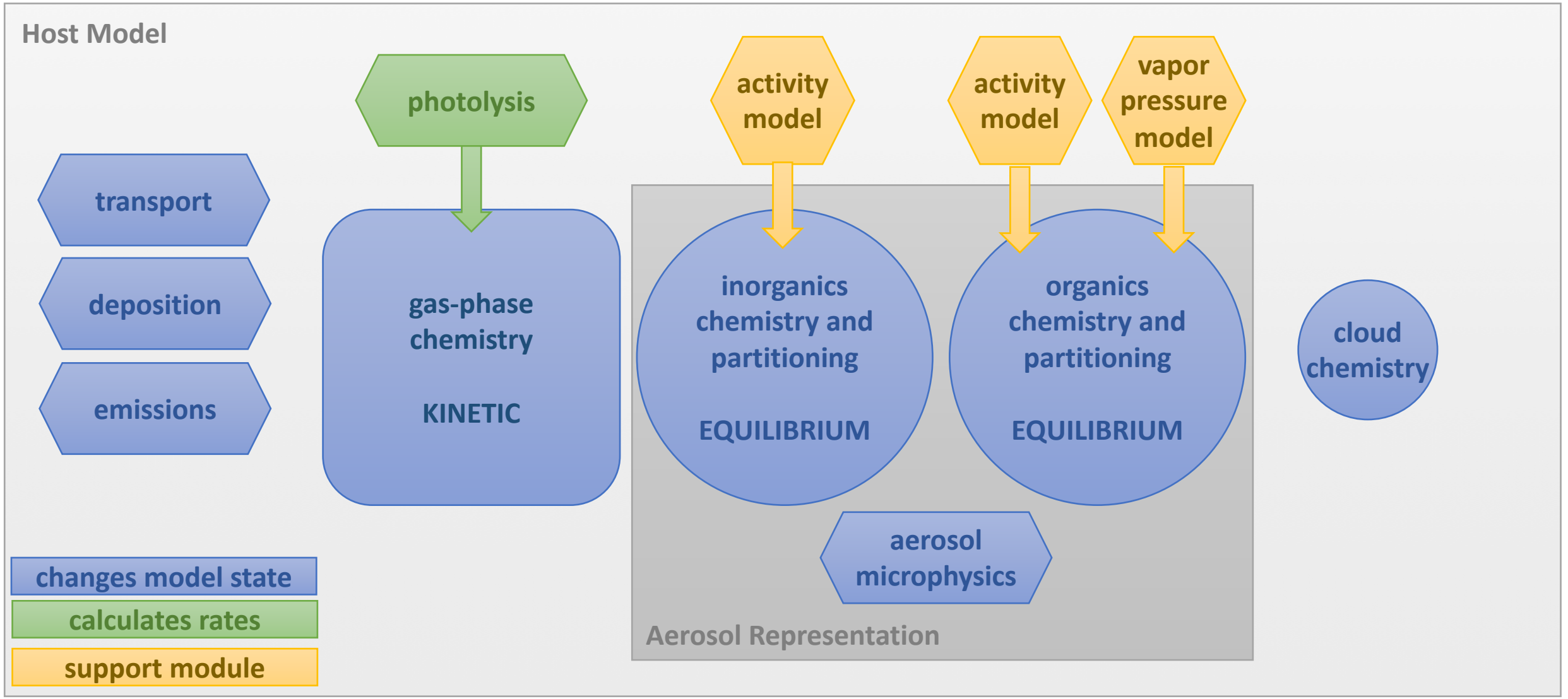
Motivation—Chemistry in Atmospheric Models

Host Model



changes model state

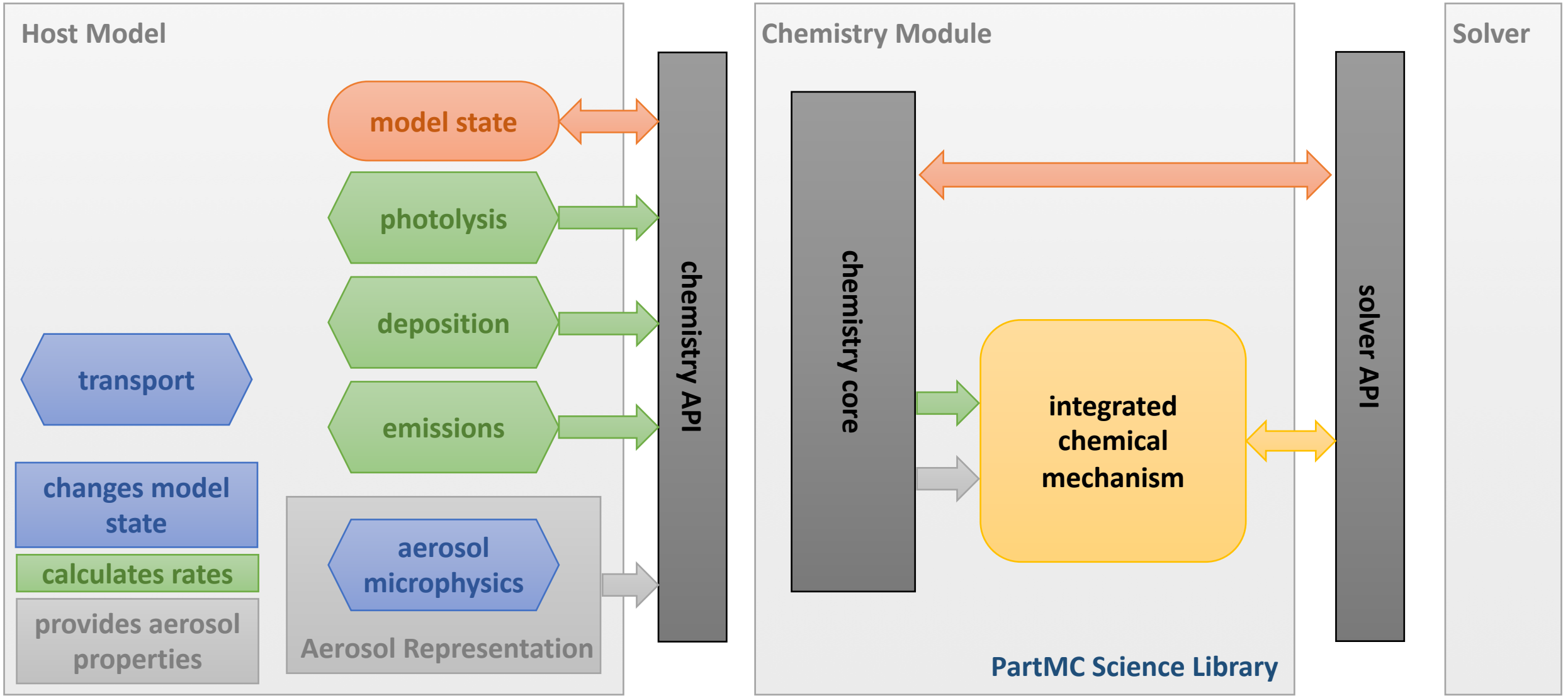
Motivation—Chemistry and Related Modules



Design Goals

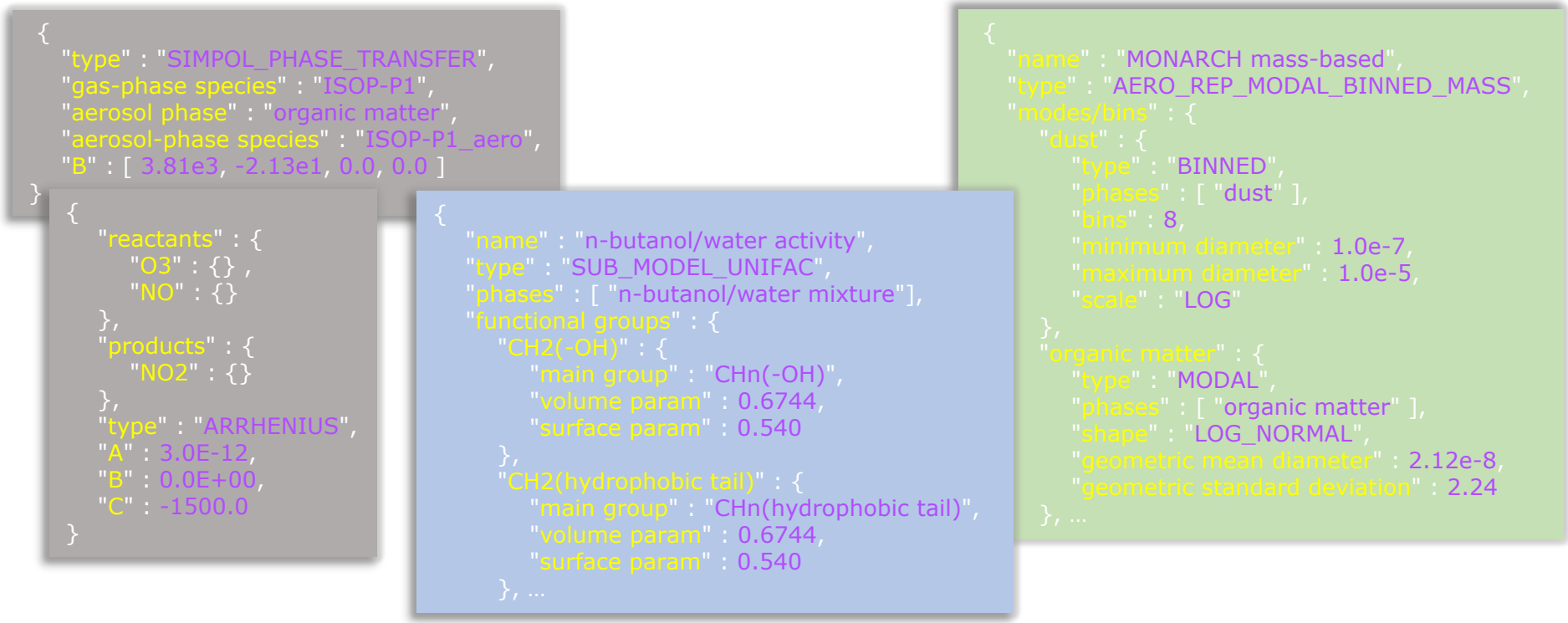
- Treat chemistry, partitioning and related processes kinetically as one system to solve
- Make it flexible
  - Usable by modelers and experimentalists
  - Portable between models (chamber, plume, regional, global)
  - Object oriented design
  - JSON configuration files
- Make it efficient
  - Scalable chemical complexity
  - Condensed data structure
  - Porting to GPUs

Approach—Integrated Chemistry Module



JSON Configuration Files

- **Readily applied to science models**
- **Industry standard – lots of free tools available**



JSON Configuration Files – Arrhenius Reaction

$$NO3 + NO \xrightarrow{k} 2\ NO2$$

$$k = Ae^{\left(\frac{C}{T}\right)}$$

```
{
 "reactants" : {
  ”NO3" : {},
  "NO" : {}
 },
 "products" : {
  "NO2" : { ”yield” : 2.0 }
 },
 "type" : "ARRHENIUS",
 "A" : 1.5E-11,
 "C" : 170.0
}
```

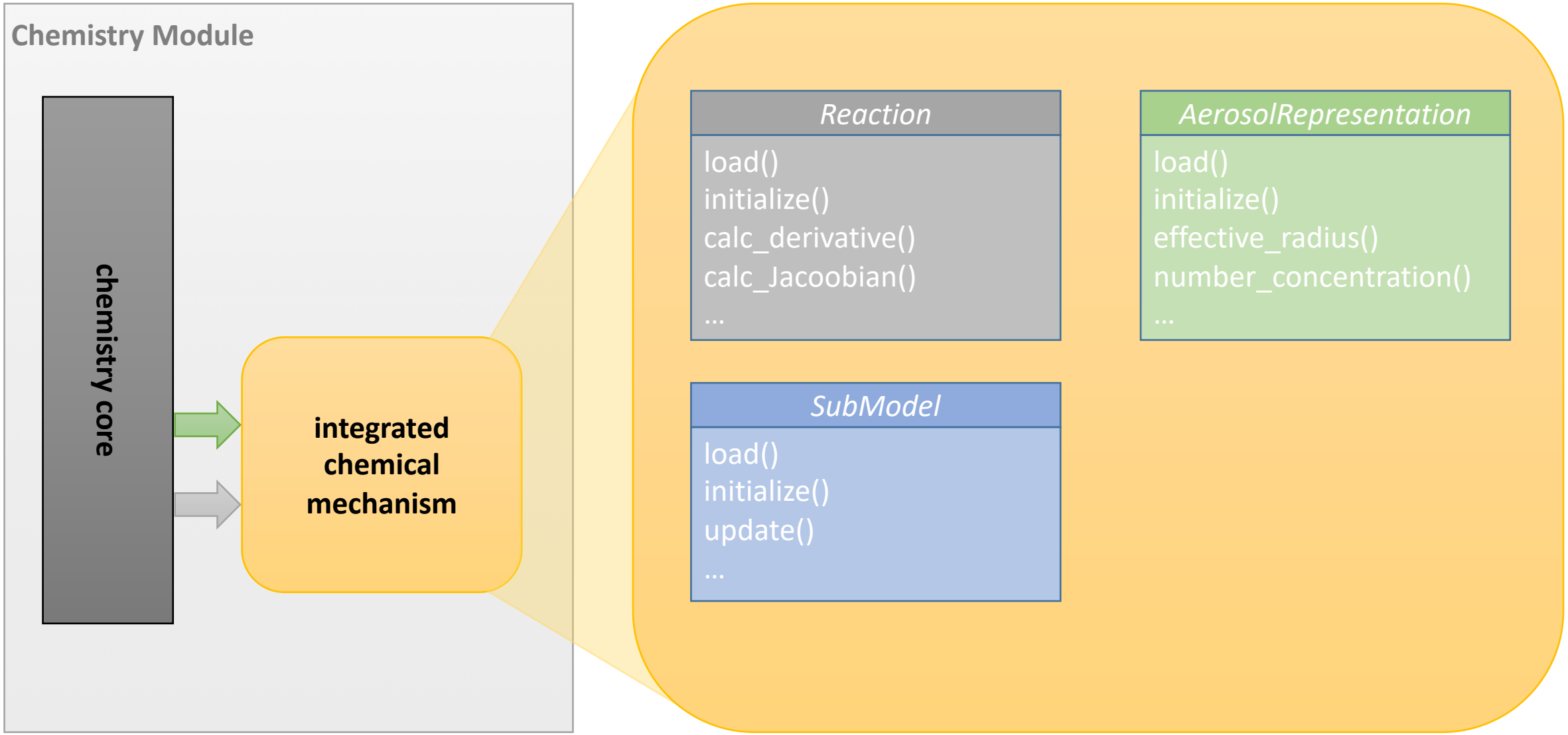
JSON Configuration Files – UNIFAC Activity

```
{
 "name" : "n-butanol/water activity",
 "type" : "SUB_MODEL_UNIFAC",
 "phases" : [ "n-butanol/water mixture"],
 ”main groups" : {
  "CHn(-OH)" : {
    "interactions with" : {
     "OH" : 986.5,
     ”H2O" : 2314
    }
  },
  "CHn(hydrophobic tail)" : {
    "interactions with" : {
     "OH" : 986.5,
     ”H2O" : 1325
    }
  }, …
```

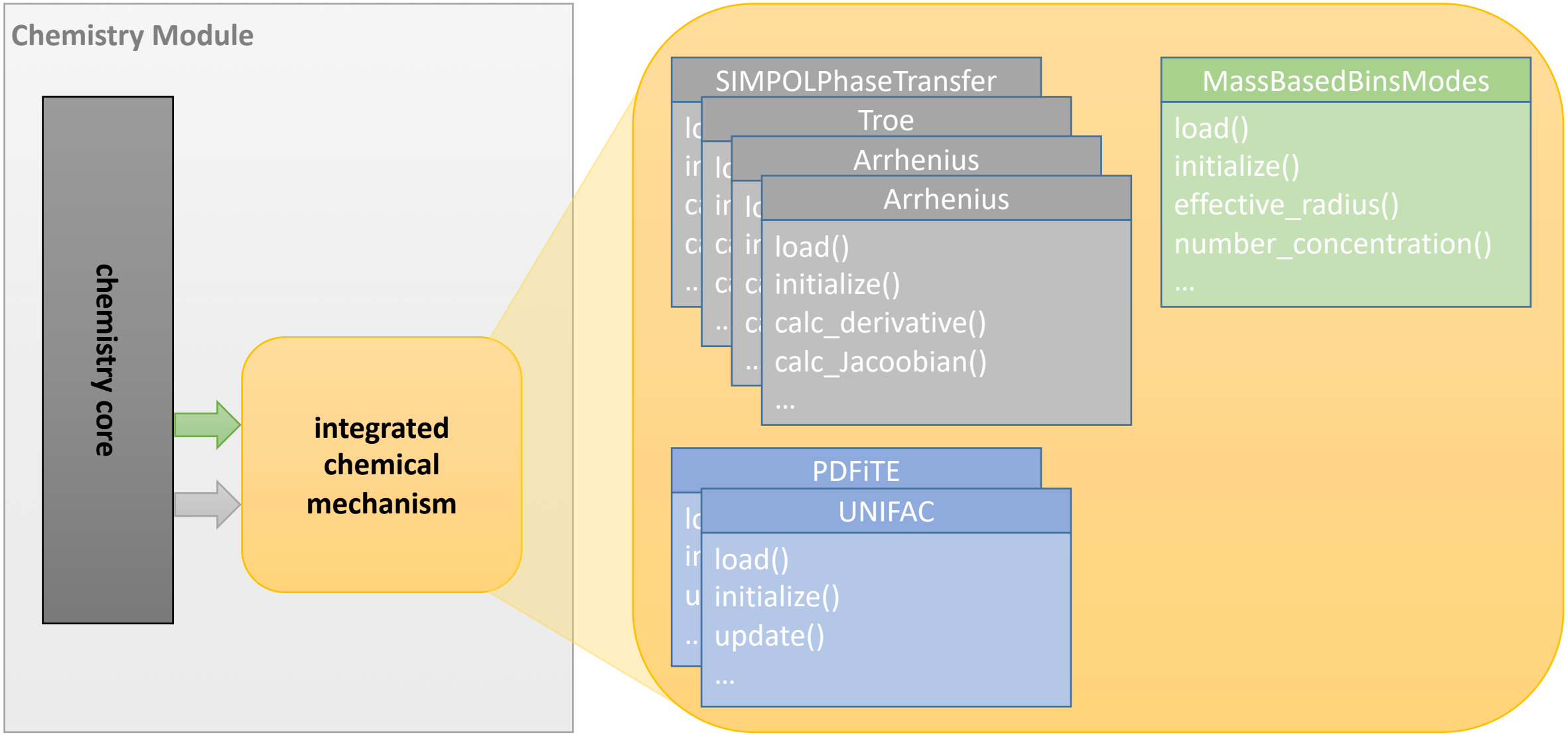
	a_{mn} (this study)				
	CH_n with -OH group	CH_n in hydrophobic tails	CH_n in alcohols	OH	H_2O
CH_n with -OH group	0.0	0.0	0.0	986.5	2314
CH_n in hydrophobic tails	0.0	0.0	0.0	986.5	1325
CH_n in alcohols	0.0	0.0	0.0	986.5	1890
OH	156.4	156.4	156.4	0.0	276.4
H_2O	−89.71	362.1	162.3	−153.0	0.0

Marcolli, C., & Peter, T. (2005). *Atmos. Chem. Phys Discuss*, *5*(2), 1501–1527.

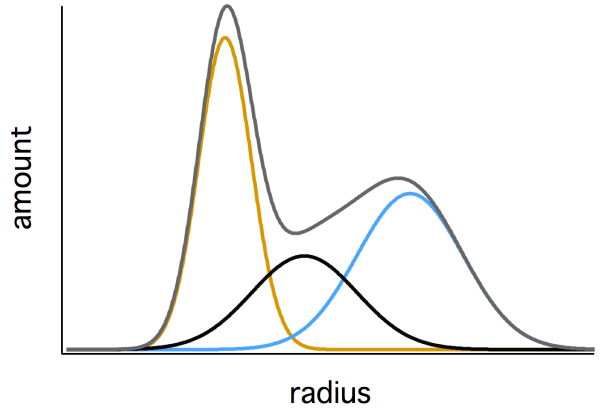
Object-Oriented Design

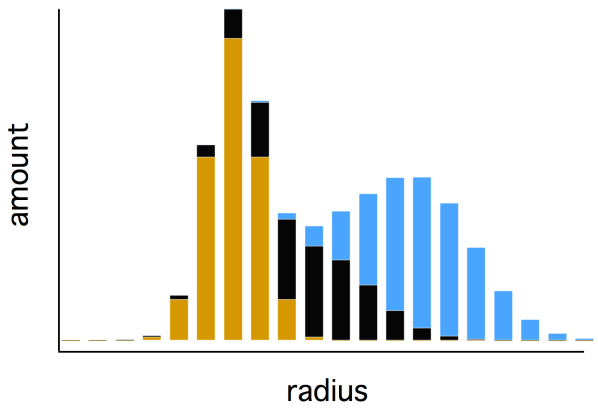


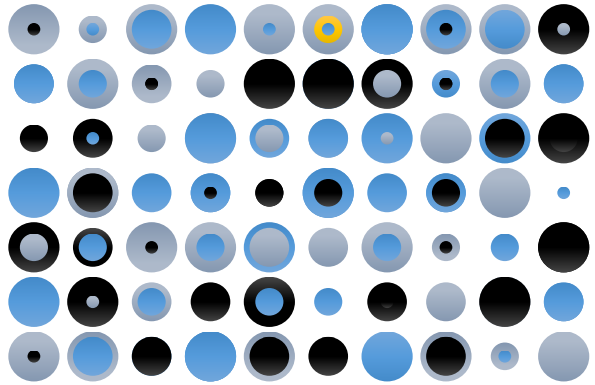
Object-Oriented Design



Aerosol Representations in Chemical Models – Challenges

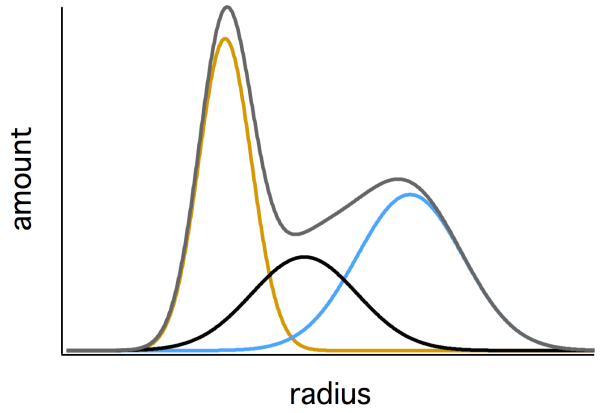






Modal **Binned** **Particle Resolved**

Aerosol Representation Abstraction – Approach



Modal

```
{
  "name" : "Modal",
  {
    "name" : "inorganics",
    {
      "name" : "black carbon",
      {
        "name" : "organics",
        "type" : "AERO_PHASE",
        "species" : [
          "PM_phob", "PM_phil", "ISOP-P1_aero",
          "ISOP-P2_aero", "TERP-P1_aero", "TERP-P2_aero"
        ]
      }
    }
  }
}
```

INPUT

Modal
load() initialize() effective_radius() number_concentration() …

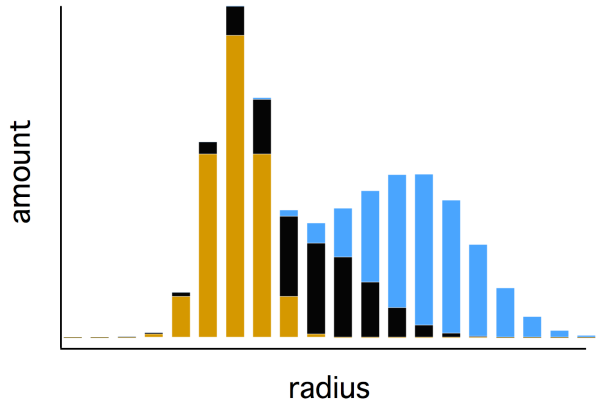
Model State

- gas-phase species
- BC — mode 1 – black carbon
- O — mode 2 – organics
- I — mode 3 – inorganics

INPUT

AerosolPhase
load() initialize() …

Aerosol Representation Abstraction – Approach



Binned

```
{
  "name" : "Modal",
  {
    "name" : "inorganics",
    {
      "name" : "black carbon",
      {
        "name" : "organics",
        "type" : "AERO_PHASE",
        "species" : [
          "PM_phob", "PM_phil", "ISOP-P1_aero",
          "ISOP-P2_aero", "TERP-P1_aero", "TERP-P2_aero"
        ]
      }
    }
  }
}
```

INPUT

Binned
load() initialize() effective_radius() number_concentration() …

Model State

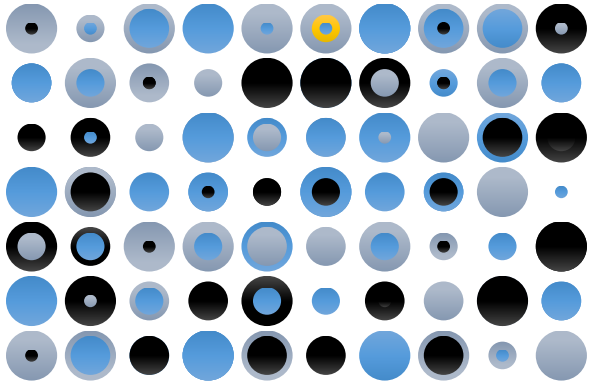
- gas-phase species
- BC bin 1 – black carbon
- O bin 1 – organics
- I bin 1 – inorganics
- BC bin 2 – black carbon
- O bin 2 – organics
- I bin 2 – inorganics
- bin 3 – …

INPUT

AerosolPhase
load() initialize() …

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Aerosol Representation Abstraction – Approach



ParticleResolved

load()
initialize()
effective_radius()
number_concentration()
…

INPUT

Model State

- gas-phase species
- BC particle 1 – black carbon
- O particle 1 – organics
- I particle 1 – inorganics
- BC particle 2 – black carbon
- O particle 2 – organics
- I particle 2 – inorganics
- particle 3 – …

Particle Resolved

```
{
  "name" : "Modal",
  {
    "name" : "inorganics",
    {
      "name" : "black carbon",
      {
        "name" : "organics",
        "type" : "AERO_PHASE",
        "species" : [
          "PM_phob", "PM_phil", "ISOP-P1_aero",
          "ISOP-P2_aero", "TERP-P1_aero", "TERP-P2_aero"
        ]
      }
    }
  }
}
```

INPUT

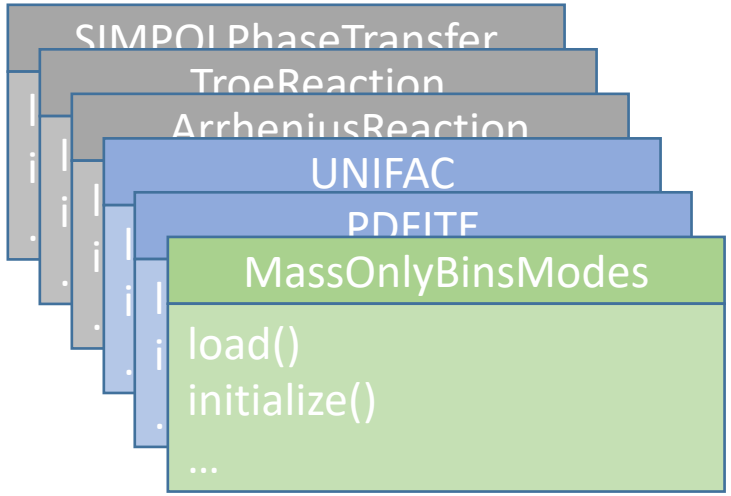
AerosolPhase

load()
initialize()
…

Work Flow – Initialization

USER

INPUT



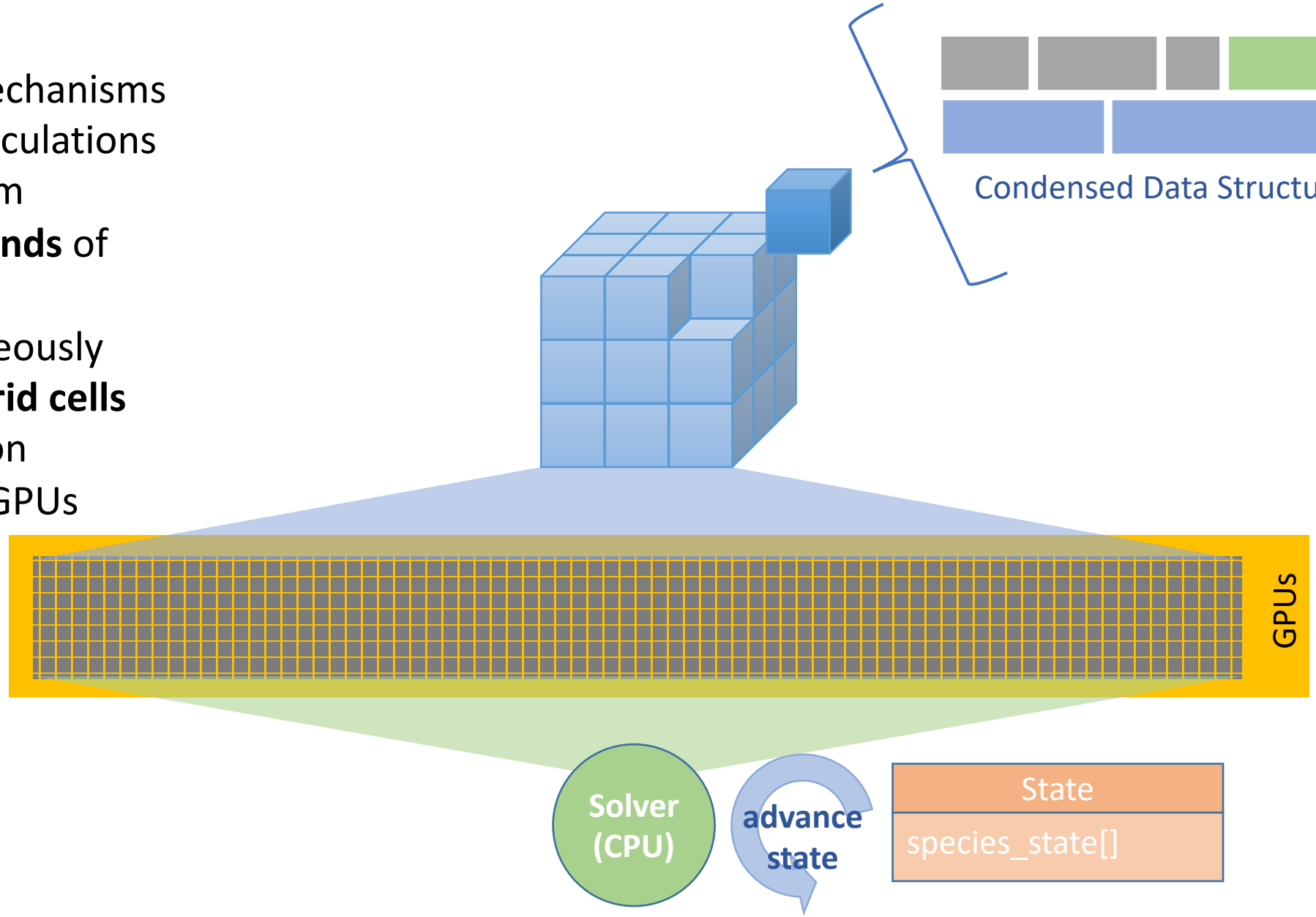
OPTIMIZE

- Single dense data block
  - Species indices
  - Fixed parameters
  - Environment-dependent parameters
  - etc.

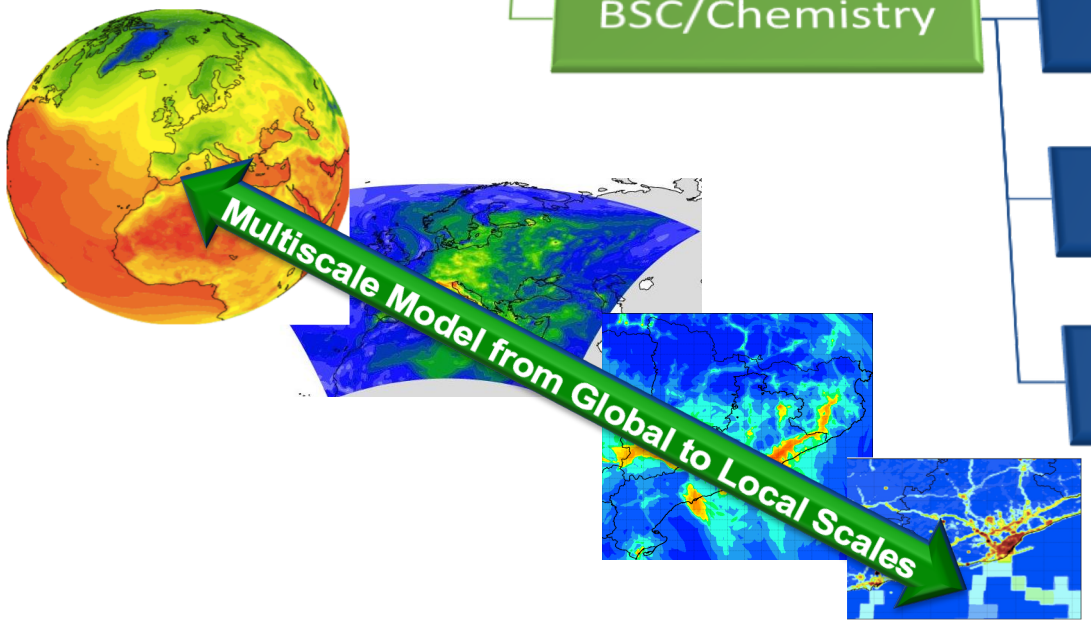
Condensed Data Structure

Porting to GPUs

- Solving chemical mechanisms involve repeated calculations of contributions from **hundreds** or **thousands** of individual **reactions**
- Approach: simultaneously solve for **multiple grid cells** by spreading reaction calculations across GPUs



MONARCH: On-line Weather–Chemistry Model

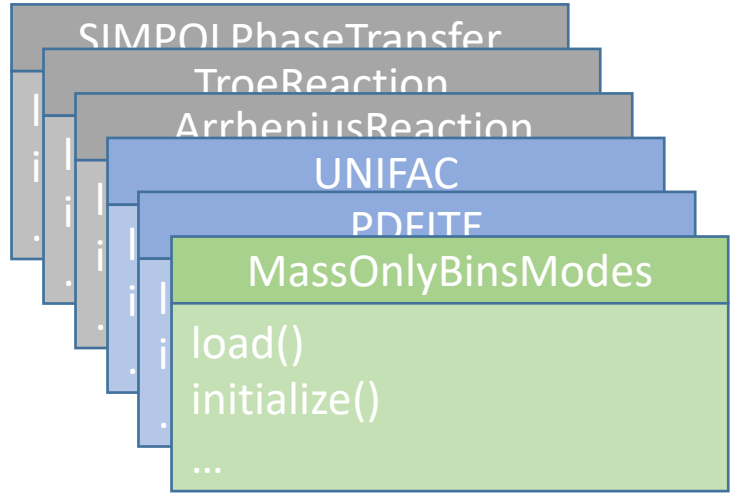


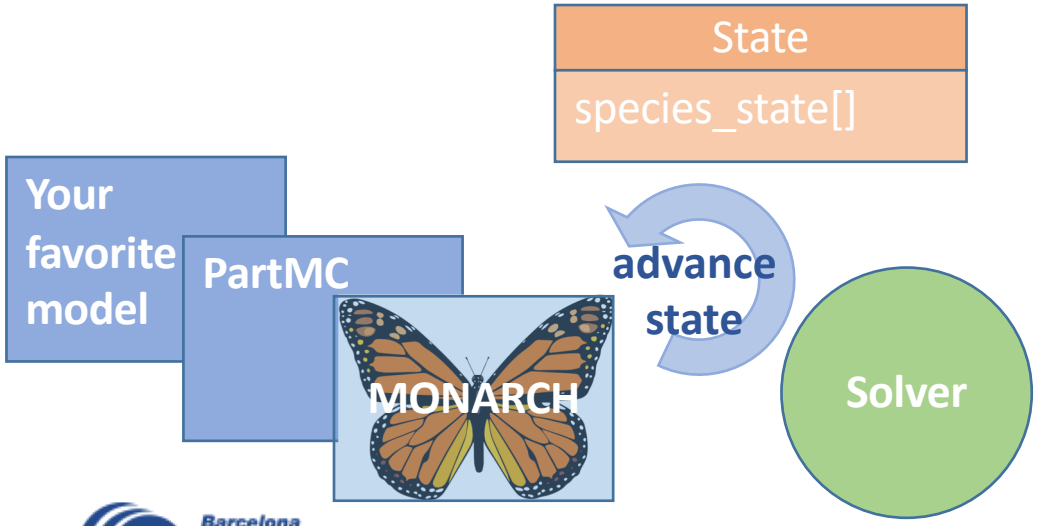
- MONARCH
  - NCEP/NMMB
    - → *Janjic and Gall (NCAR/TN 2012)*
    - → *Janjic and Vasic (EGU2012)*
    - → *Janjic et al. (MWR 2011)*
    - → *(...)*
  - BSC/Chemistry
    - AEROSOLS
      - → *Pérez et al. (ACP 2011)*
      - → *Haustein et al. (ACP 2012)*
      - → *Spada et al. (ACP 2013)*
      - → *Spada et al. (AE 2014)*
      - → *Spada (2015)*
      - → *DiTomaso et al. (GMD 2017)*
    - VOLCANIC ASH
      - → *Martí et al. (ACP 2016)*
    - GAS-PHASE CHEMISTRY
      - → *Jorba et al. (JGR 2012)*
      - → *Badia and Jorba (AE 2014)*
      - → *Badia et al. (GMD 2017)*

Chemistry Module – Overall Workflow

- Change the chemical mechanism ***without recompiling***
  - Vary mechanism complexity based on conditions/location
  - Compare mechanisms in real time
- Use ***same mechanisms*** across models (MONARCH, PartMC, etc.) changing only Aerosol Representation JSON

Load input files into model objects





Condensed Data Structure

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

The PartMC library is available at: `https://github.com/compdyn/partmc`

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Thank you

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 747048.

matthew.dawson@bsc.es

Check out our on-going development!

With Docker© installed:

```
> git clone https://github.com/compdyn/partmc.git
> cd partmc
> git checkout chem_mod
> docker build -t try-out-chemistry .
> docker run -it try-out-chemistry bash
> cd build
> make test
```

```
      Start 13: test_rxn_first_order_loss
13/85 Test #13: test_rxn_first_order_loss .............   Passed    0.06 sec
      Start 14: test_rxn_HL_phase_transfer
14/85 Test #14: test_rxn_HL_phase_transfer .............   Passed    0.07 sec
      Start 15: test_rxn_PDFiTE_activity
15/85 Test #15: test_rxn_PDFiTE_activity ...............   Passed    0.04 sec
      Start 16: test_rxn_photolysis
16/85 Test #16: test_rxn_photolysis ....................   Passed    0.06 sec
...
      Start 21: test_sub_model_UNIFAC
21/85 Test #21: test_sub_model_UNIFAC ..................   Passed    0.03 sec
...
      Start 23: test_chemistry_cb05cl_ae5
23/85 Test #23: test_chemistry_cb05cl_ae5 ..............   Passed    5.78 sec
      Start 25: test_MONARCH_1
25/85 Test #25: test_MONARCH_1 .........................   Passed    0.37 sec
      Start 26: test_MONARCH_2
26/85 Test #26: test_MONARCH_2 .........................   Passed    7.00 sec
```